

USER SCIENCE DIVISION REPORT

Chi-Chang Kao

Associate Chair for User Science

Organization and Mission

The User Science Division (USD) coordinates major facility activities related to users so that we can be more effective in communicating with the user community, strengthening existing scientific programs, fostering the growth of new scientific programs, and raising the visibility of the exciting science produced by our users both inside and outside the scientific community. The division consists of five sections: User Administration (Kathy Nasta), Information and Outreach (Lisa Miller), Beamline Development and Support (Steve Hulbert), Scientific Program Support (Ron Pindak), and Detectors and Controls (Peter Siddons). The major initiatives and accomplishments of the User Science Division and the NSLS user community for 2006 are summarized below.

2006 Activities

NSLS Five-Year Plan

The most important activity of the USD in 2006 was the development of the NSLS Five-Year Strategic Plan. We worked closely with the user community and the NSLS Science Advisory Committee (SAC) to identify future scientific opportunities, as well as beamline and infrastructure upgrades needed to exploit those opportunities. A more detailed plan, which includes the resources required, funding sources, and schedule to implement these upgrades, also was developed.

Contributing User Proposals

With the assistance from the SAC, the first set of nine Contributing User (CU) proposals was ap-

proved. The approved CUs include two research resources: COMPRES (a National Science Foundation-funded research resource for earth sciences) and PXRR (a National Institutes of Health and DOE Office of Biological and Environmental Research-funded resource for macromolecular crystallography), as well as several groups of researchers who bring significant new instrumentation to the NSLS. Although these CU programs have only been in operation for a relatively short time, they have already made a significant impact to the NSLS user science program.

Funding Renewed for X6A

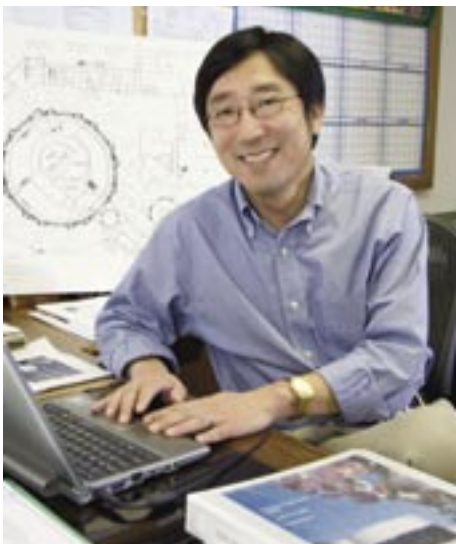
On the scientific program front, we are delighted that funding for the East Coast Structural Biology Facility, beamline X6A, has been renewed by the National Institute of General Medical Sciences (NIGMS). X6A is funded for macromolecular crystallography and, in particular, to provide beam time access to young scientists in the process of establishing research groups whose primary interest is not x-ray crystallography. This grant from NIGMS has enabled the NSLS to significantly expand its structural biology program, as well as to develop a rapid access and remote user program.

NSLS, BNL to Build Linac Coherent Light Source Detectors

The NSLS and Brookhaven's Instrumentation Division were awarded a multi-year project to construct detectors for the Linac Coherent Light Source (LCLS) project at the Stanford Linear Accelerator Center (SLAC). This is a very challenging project and an important milestone for the detector development effort at the NSLS. It will significantly expand the expertise of the detector and control group at the NSLS, led by Peter Siddons, which has successfully delivered a wide range of detectors to users over the last several years, including fast photon counting detectors and linear array detectors. The detectors developed for the LCLS will also benefit many scientific programs at the NSLS.

Education and Outreach

We continue to put a large focus on user education, training, and outreach at the NSLS. In the area of user training, our annual XAFS short course was held in October 2006, with the title "Short Course: XAFS Studies of Nanocatalysis and Chemical Transformations." In addition, two macromolecular crystallography courses, "Rapi-Data 2006," and the "X6A Workbench: Advanced Tools for Structural Biology," continued to attract a large number of users. We also worked closely with users to organize additional focused scien-



Chi-Chang Kao

tific workshops, including "Synchrotron Catalysis Consortium: New Opportunities for in situ XAFS Studies of Catalysis," a workshop on "Soft Matter and Biomolecular Materials: X-ray Scattering Enabled by High Brightness Beamlines," the "Nanoscale Correlations Heterostructures" workshop, a workshop on "Chemical and Biological Applications of X-ray Emission Spectroscopy," a workshop on "Platforms for the Integration of Biological Systems into Nanomaterials and Interfaces," a "Vacuum Ultraviolet Radiometry" workshop, and the workshop "Crystallization: Focus on Optimization and High Throughput Techniques." These short courses and workshops were very effective in introducing the use of synchrotron techniques in a particular area of science to non-synchrotron users. Many new research opportunities and collaborations have resulted from them. Additionally, we've continued our effort this year to coordinate closely with the Center for Functional Nanomaterials in order to reach out to nanoscience researchers through joint seminars, workshops, and visits to interested universities and institutions.

Beamline Upgrades and Performance Improvements

We initiated a program this year to characterize beamline performance, including flux, energy resolution, and focal spot size, on a regular basis, led by Lonny Berman. The goal is to establish a performance baseline for all NSLS facility beamlines, and identify areas that need improvement. In addition, the three major upgrade projects initiated and completed this year by the NSLS and PRTs were at X18, X25, and X9. Details are described below:

X18B Beamline Upgrade for Quick-EXAFS

A new monochromator drive and data-collection scheme have been developed for beamline X18B to allow quick measurements of x-ray absorption spectra (QEXAFS). The micrometer on the standard NSLS tangent-arm driven monochromator has been replaced with a cam, which continuously changes the Bragg-angle of the monochromator with a simple rotation of a motor. Different positions in the cam result in different angular ranges over which the monochromator is rotated, which translates into different energy ranges for the scans. This allows the user to concentrate on either the near-edge structure (XANES), or the extended fine structure (EXAFS). The data are collected using an analog-to-digital converter, which digitizes the voltage from the current amplifier directly.

During 2006, the QEXAFS setup was used by three groups. Switching the X18B monochromator control system from conventional EXAFS to QEXAFS mode takes only minutes. The graphical user interface (GUI) for QEXAFS data collection is now capable of continuous operation with data

collection duration of one or five minutes, each with many cycles. In fast mode, a full EXAFS scan with good signal to noise ratio can be collected in 200 milliseconds. This new capability will enable the use of x-ray absorption spectroscopy for fast in-situ kinetic measurements, e.g., for catalysis and fuel cell research.

X25 Cryo-Capable Mini-Gap In-Vacuum Undulator Installed in the X-Ray Ring

At the start of 2004, beamline X25's programmatic focus shifted completely to monochromatic macromolecular crystallography, following 14 years of operation as a mixed-use high-brightness beamline. Thus, the NSLS was presented with an opportunity to renovate the beamline, as well as the radiation source, to optimize them for a dedicated macromolecular crystallography program. To this end, the BNL Macromolecular Crystallography Research Resource (PXRR), a collaboration between the BNL Biology Department and the NSLS, submitted a funding request in late 2002 as part of its proposal to the National Institutes of Health's National Center for Research Resources and the Department of Energy's Office of Biological and Environmental Research (DOE BER) to renew its five-year grant. The proposal was well received, and \$2.2M in funds was awarded by DOE BER beginning in late 2003, to be dispensed over the course of three fiscal years.



The newly installed double crystal monochromator at beamline X25 is shown, with its vacuum chamber open. The white beam enters from the right and the diffracted beam emerges to the left. The first silicon crystal is mounted on a copper support that can be cooled to cryogenic temperature, and the second crystal is mounted in a bender that can curve the crystal sagittally in order to focus the beam horizontally. Directly beneath the monochromator is the cryocooler and heat exchanger assembly which forms part of the new cryogenic refrigerator for cooling the first crystal.



The new X25 MGU installed in the NSLS x-ray ring.

During the December 2005 shutdown, the original hybrid wiggler, which served as the radiation source for beamline X25 since its inception in 1990, was replaced by a custom-designed in-vacuum miniature-gap hybrid undulator. At a photon energy of 6.3 keV, the new radiation source will be 15 times brighter than the old one, and will be six times brighter at a photon energy of 10.5 keV. Its design consists of 0.99 meter-long planar hybrid magnet arrays with a period length of 18 mm (55 periods total) and a minimum attainable gap of 5.6 mm, with a corresponding maximum deflection parameter, K , of 1.5. The NdFeB-type



X-ray burns taken using original wiggler (top) and the new undulator (bottom), in the same location, show that the undulator beam is much smaller than the wiggler beam, as expected.

permanent magnet material, which has been used in this insertion device, can have a higher magnetic field and a higher radiation resistance simply by cooling: Operation at 150K will likely produce a 13-14% higher magnetic field (and higher K), resulting in a larger photon energy tuning range. Therefore, this undulator design

also incorporates a provision for cryogenic operation, which might be pursued in the future. Unlike previous miniature-gap undulator designs in use at the NSLS, the one now implemented for X25 will be continuously tunable from 2 to 20 keV by employing all harmonics up through the 9th. The undulator vacuum and gap separation system was manufactured by Advanced Design Consulting of Lansing, NY. In conjunction with the installation of the undulator, certain components in the front end of the beamline, and the active interlock system that protects the x-ray ring exit chamber, were upgraded in order to cope with the much higher power density of the undulator beam.

In addition to the new radiation source, upgrades to the beamline optics also were implemented in order to exploit the properties of the new source. The current double crystal monochromator was replaced by one that incorporates cryogenic cooling of the first crystal and sagittal bending of the second crystal to permit horizontal focusing. It was followed by the installation of a new bendable mirror, containing multiple coating stripes, to permit vertical focusing. The completion of the X25 upgrade, expected in FY07, is essential to the macromolecular crystallography program at the NSLS.

X9 to X3 Beamline Relocation Complete

In October 2006, beamlines X3A and X3B began operating without restrictions after being transferred from X9 in just four and a half months. The relocation of the two beamlines was completed in advance of original estimates, with deconstruction of X9A and X9B beginning in early May and the first commissioning beams at X3A and X3B running in late August and early September.

The Case Center for Synchrotron Biosciences, which utilized the former X9 beamlines, moved to X3 to make room for a new undulator-based beamline at X9. The X9 straight section is cur-



Beamline X3 before



Beamline X3 after

rently the last one available in the x-ray ring. It will be used for a small-angle x-ray scattering Facility Beamline with BNL's Center for Functional Nanomaterials as a Contributing User. The new X9 beamline is expected to be operational in 2008, with commissioning completed during the first cycle of the year and full operations starting in May or June.

Although performed quickly, the relocation from X9 to X3 wasn't an easy process. First, the X16C beamline was renovated to accept the experimental program that was operating at beamline X3B1. Next, the former X3 beamlines and experimental equipment were completely removed from the X3 floor space. Then, planning, surveying, and engineering and design for the relocation of the two X9 bending magnet beamlines to counterpart locations at X3 were undertaken and the necessary reviews were completed. The X9A hutch was modified and re-built in its new location at X3A, a new hutch for X3B was constructed, and associated utilities and interlocks were installed. The beam pipes for both beamlines, which penetrate the shield wall and connect them with the front end, were moved from X9 to X3, and the shield wall and neighboring lead shields were re-built accordingly. All experimental equipment and controls for these beamlines also were moved to their new locations at X3.

All of the equipment was in place at X3 by August, with the first commissioning beams running shortly after. Re-commissioning was completed around the end of the 2006 fiscal year. In addition to hosting Participating Research Team (PRT) experiments, both beamlines also are accepting General Users.